

## Laboratory:Materials Design by Computer Simulation 2000-2004

著者	Institute for Materials Research, Tohoku University
journal or publication title	List of Publications 2000-2004
URL	<a href="http://hdl.handle.net/10097/56473">http://hdl.handle.net/10097/56473</a>

Guo, Y; Gu, BL; Kawazoe, Y

*Tunneling transport of two-dimensional spin-electrons through magnetic quantum structures*

Acta Phys. Sin. 49 (2000) 1814 – 1820

00-IMR0222

Belosludov, VR; Shpakov, VP; Tse, JS; Belosludov, RV; Kawazoe, Y

*Mechanical stability of gas hydrates under pressure*

Ann. NY Acad.Sci. 912 (2000) 993 – 1002

00-IMR0223

Wu, J; Duan, WH; Gu, BL; Yu, JZ; Kawazoe, Y

*Finite size effects in carbon nanotubes*

Appl. Phys. Lett. 77 (2000) 2554 – 2556

00-IMR0224

Ohno, K; Kawazoe, Y

*A modified CCA model describing gelation processes*

Comput. Theor. Polym. Sci. 10 (2000) 269 – 274

00-IMR0225

Shida, K; Ohno, K; Kimura, M; Kawazoe, Y

*Monte Carlo analysis of the osmotic pressure of athermal polymer solutions in dilute and semi-dilute regimes*

Comput. Theor. Polym. Sci. 10 (2000) 281 – 285

00-IMR0226

Parlinski, K; Kawazoe, Y

*Ab initio study of phonons in the rutile structure of SnO<sub>2</sub> under pressure*

Eur. Phys. J. B 13 (2000) 679 – 683

00-IMR0227

Parlinski, K; Kawazoe, Y

*Ab initio study of phonons and structural stabilities of the perovskite-type MgSiO<sub>3</sub>*

Eur. Phys. J. B 16 (2000) 49 – 58

00-IMR0228

Mizuseki, H; Kawazoe, Y

*Simulation of electrochemical deposition process by a multiparticle diffusive aggregation model*

J. Appl. Phys. 87 (2000) 4611 – 4616

00-IMR0229

Mizuseki, H; Jin, Y; Kawazoe, Y; Wille, LT

*Growth processes of magnetic clusters studied by direct simulation Monte Carlo method*

J. Appl. Phys. 87 (2000) 6561 – 6563

00-IMR0230

Guo, Y; Wang, H; Gu, BL; Kawazoe, Y

*Spin-polarized transport through a ZnSe/Zn<sub>1-x</sub>MnxSe heterostructure under an applied electric field*

J. Appl. Phys. 88 (2000) 6614 – 6617

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Ohtsuki, T; Ohno, K; Shiga, K; Kawazoe, Y; Maruyama, Y; Masumoto, K <i>Systematic study of foreign-atom-doped fullerenes by using a nuclear recoil method and their MD simulation</i> J. Chem. Phys. 112 (2000) 2834 – 2842	00-IMR0232
Parlinski, K; Lazewski, J; Kawazoe, Y <i>Ab initio studies of phonons in MgO by the direct method including LO mode</i> J. Phys. Chem. Solids 61 (2000) 87 – 90	00-IMR0233
Guo, Y; Wang, B; Hu, H; Yu, JZ; Gu, BL; Kawazoe, Y <i>Spin-dependent electronic states and magnetoconductance in a magnetic quantum antidot</i> J. Phys.-Condes. Matter 12 (2000) 3359 – 3367	00-IMR0234
Shida, K; Ohno, K; Kimura, M; Kawazoe, Y <i>Monte Carlo study of the second virial coefficient and statistical exponent of star polymers with large numbers of branches</i> Macromolecules 33 (2000) 7655 – 7662	00-IMR0235
Shiga, K; Ohno, K; Kawazoe, Y; Maruyama, Y; Hirata, T; Hatakeyama, R; Sato, N <i>Ab initio molecular dynamics simulation for the insertion process of Si and Ca atoms into C-74</i> Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process. 290 (2000) 6 – 10	00-IMR0236
Tsunekawa, S; Sahara, R; Kawazoe, Y; Kasuya, A <i>Origin of the blue shift in ultraviolet absorption spectra of nanocrystalline CeO<sub>2-x</sub> particles</i> Mater. Trans. JIM 41 (2000) 1104 – 1107	00-IMR0242
Yu, JZ; Sun, Q; Wang, Q; Onose, U; Akiyama, Y; Kawazoe, Y <i>First-principles calculation on dissociation of hydrogen molecule in nickel</i> Mater. Trans. JIM 41 (2000) 1114 – 1117	00-IMR0243
Wu, J; Gu, BL; Yu, JZ; Kawazoe, Y <i>Coherent transport through carbon nanotubes with finite length</i> Mater. Trans. JIM 41 (2000) 571 – 573	00-IMR0237
Wang, JT; Zhou, L; Wang, DS; Kawazoe, Y <i>Ab initio-Monte Carlo studies on the finite-temperature properties of L1(0) FeAu superlattice</i> Mater. Trans. JIM 41 (2000) 601 – 604	00-IMR0238
Yu, JZ; Sun, Q; Wang, Q; Onose, U; Akiyama, Y; Kawazoe, Y <i>Effect of magnetic transition on hydrogen solubility in Ni</i> Mater. Trans. JIM 41 (2000) 621 – 623	00-IMR0239

Morisato, T; Ohno, K; Kawazoe, Y; Kusunoki, I <i>Study on local structures of C<sub>x</sub>N<sub>1-x</sub> films by first-principles 1s orbital energy calculations</i> Mater. Trans. JIM 41 (2000) 628 – 630	00-IMR0240
Taneda, A; Kawazoe, Y <i>Ground state structures of neutral and charged Ti clusters containing 2 to 16 atoms</i> Mater. Trans. JIM 41 (2000) 635 – 638	00-IMR0241
Mizuseki, H; Tanaka, K; Ohno, K; Kawazoe, Y <i>A new crystal growth model based on a stochastic method under an external field</i> Model. Simul. Mater. Sci. Eng. 8 (2000) 1 – 11	00-IMR0244
Sluiter, MHF; Kawazoe, Y <i>Prediction of solution enthalpies of substitutional impurities in aluminium</i> Model. Simul. Mater. Sci. Eng. 8 (2000) 221 – 232	00-IMR0245
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Onoe, J; Nakayama, T; Nakao, A; Hashi, Y; Esfarjani, K; Kawazoe, Y; Aono, M; Takeuchi, K <i>In situ FTIR, XPS, and STM studies of the nano-structure of a photopolymerized C-60 film</i> Mol. Cryst. Liquid Cryst. 340 (2000) 689 – 694	00-IMR0247
Oku, T; Schmid, G; Suganuma, K; Sun, Q; Kawazoe, Y <i>Structure of Pd-intercalated graphite onions formed by electron beam irradiation</i> Mol. Cryst. Liquid Cryst. 340 (2000) 95 – 100	00-IMR0248
Wang, Q; Sun, Q; Yu, JZ; Hashi, Y; Kawazoe, Y <i>First-principles studies on magnetism of Ni clusters coated and alloyed with Pd</i> Phys. Lett. A 267 (2000) 394 – 402	00-IMR0249
Wang, Q; Sun, Q; Yu, JZ; Gu, BL; Kawazoe, Y; Hashi, Y <i>Structures of magic Ba clusters and magic Ba suboxide clusters</i> Phys. Rev. A 62 (2000) Art. No. 063203 –	00-IMR0250
Guo, Y; Wang, H; Gu, BL; Kawazoe, Y <i>Electric-field effects on electronic tunneling transport in magnetic barrier structures</i> Phys. Rev. B 61 (2000) 1728 – 1731	00-IMR0251

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Nagai, Y; Hasegawa, M; Tang, Z; Hempel, A; Yubuta, K; Shimamura, T; Kawazoe, Y; Kawai, A; Kano, F <i>Positron confinement in ultrafine embedded particles: Quantum-dot-like state in an Fe-Cu alloy</i> Phys. Rev. B	61 (2000)	6574 – 6578	00-IMR0253
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Guo, Y; Gu, BL; Zeng, Z; Yu, JZ; Kawazoe, Y <i>Electron-spin polarization in magnetically modulated quantum structures</i> Phys. Rev. B	62 (2000)	2635 – 2639	00-IMR0255
Tsunekawa, S; Ito, S; Mori, T; Ishikawa, K; Li, ZQ; Kawazoe, Y <i>Critical size and anomalous lattice expansion in nanocrystalline BaTiO3 particles</i> Phys. Rev. B	62 (2000)	3065 – 3070	00-IMR0256
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Sun, Q; Sakurai, M; Wang, Q; Yu, JZ; Wang, GH; Sumiyama, K; Kawazoe, Y <i>Geometry and electronic structures of magic transition-metal oxide clusters M9O6 (M = Fe, Co, and Ni)</i> Phys. Rev. B	62 (2000)	8500 – 8507	00-IMR0258
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*Magnetic phase competing in MnAu systems*

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*Structural deformation of single-walled carbon nanotubes and fullerene encapsulation due to magnetized-plasma ion irradiation*

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*Asymmetry and separation of spin tunneling time in ZnSe/Zn<sub>1-x</sub>MnxSe multilayers*

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Zeng, Z; Mizuseki, H; Simamura, K; Fukuda, T; Higashino, K; Kawazoe, Y

*Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity*

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